Electronic Supplementary Material (ESI) for Dalton Transactions.

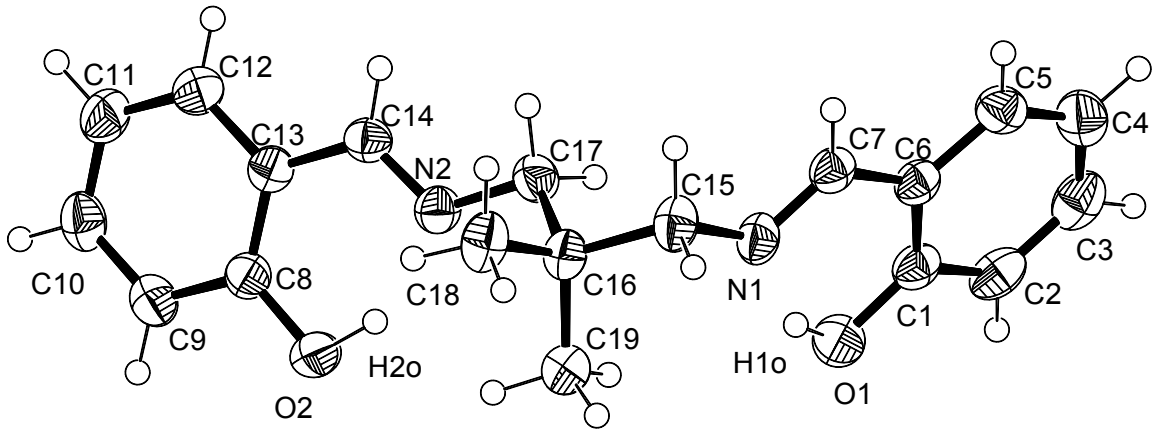

Fig 1S: C-bound hydrogen atoms were refined in idealized positions (riding model), the OH hydrogen atoms were located as residual electron density peaks and refined isotropically without any restraints.

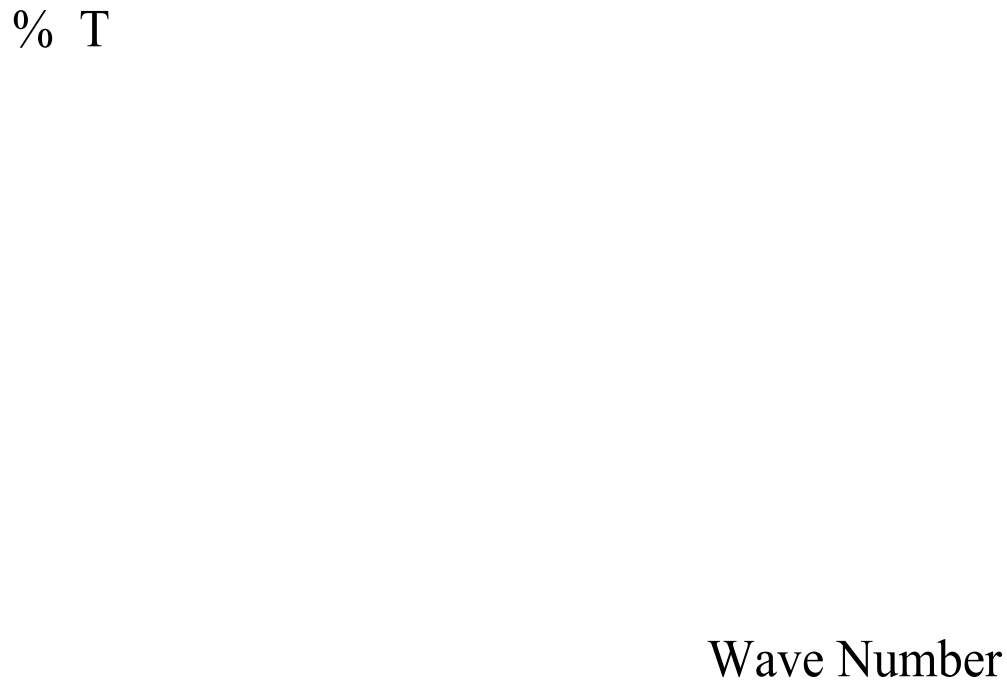

Fig 2S: IR Spectra of ligand, H_2L and its uranyl complex

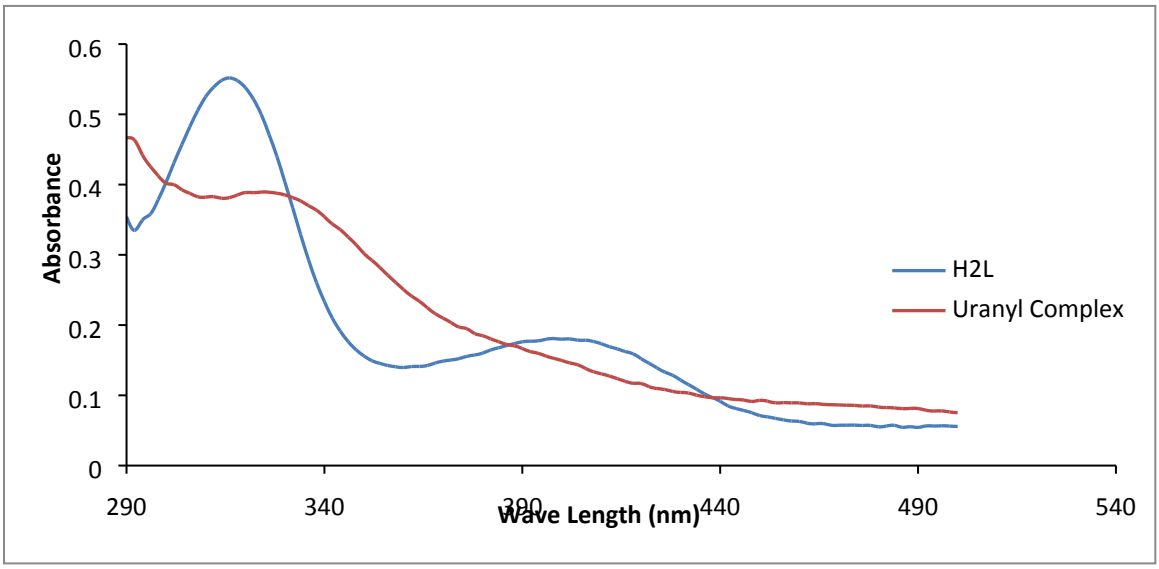

Fig 3S: Absorption spectra of ligand,H_2L and its corresponding uranyl complex

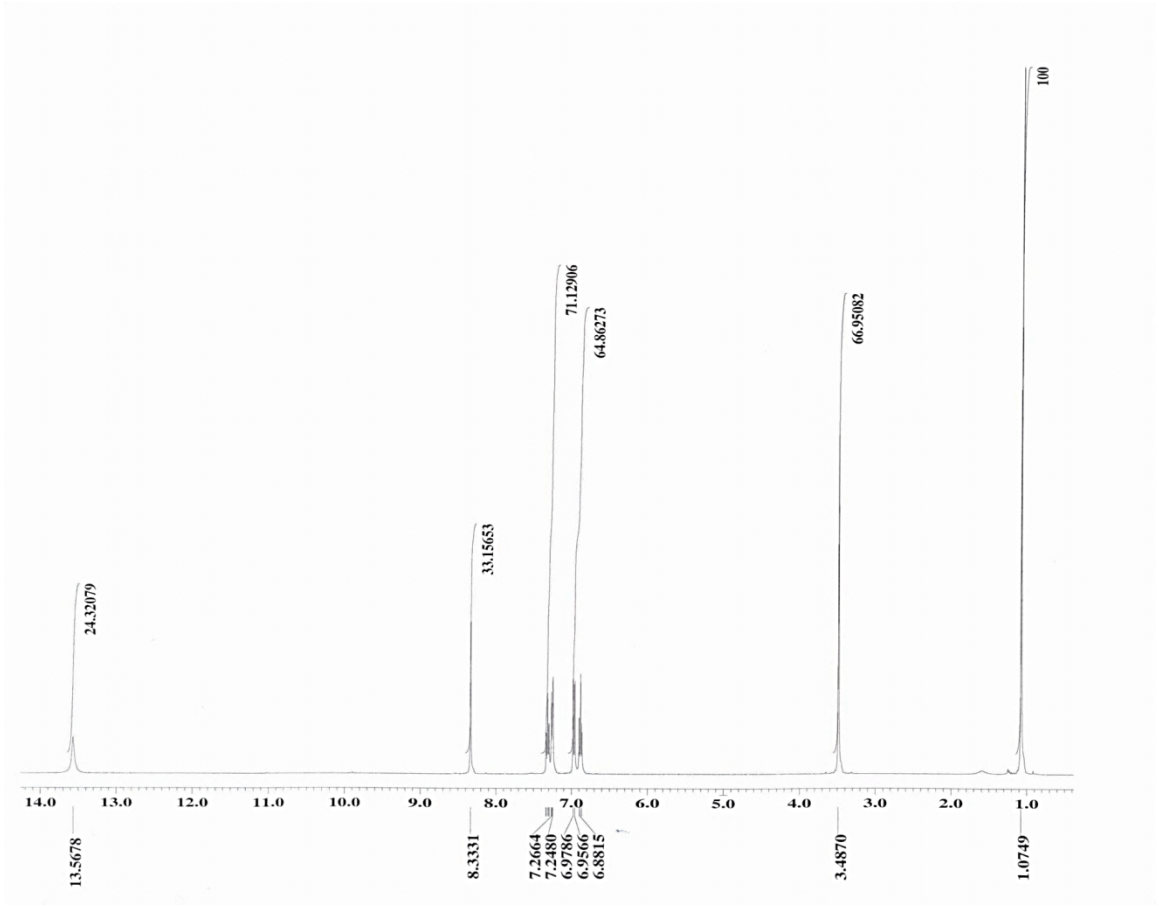

Fig 4S: ^{1}H NMR of ligand, H_2L

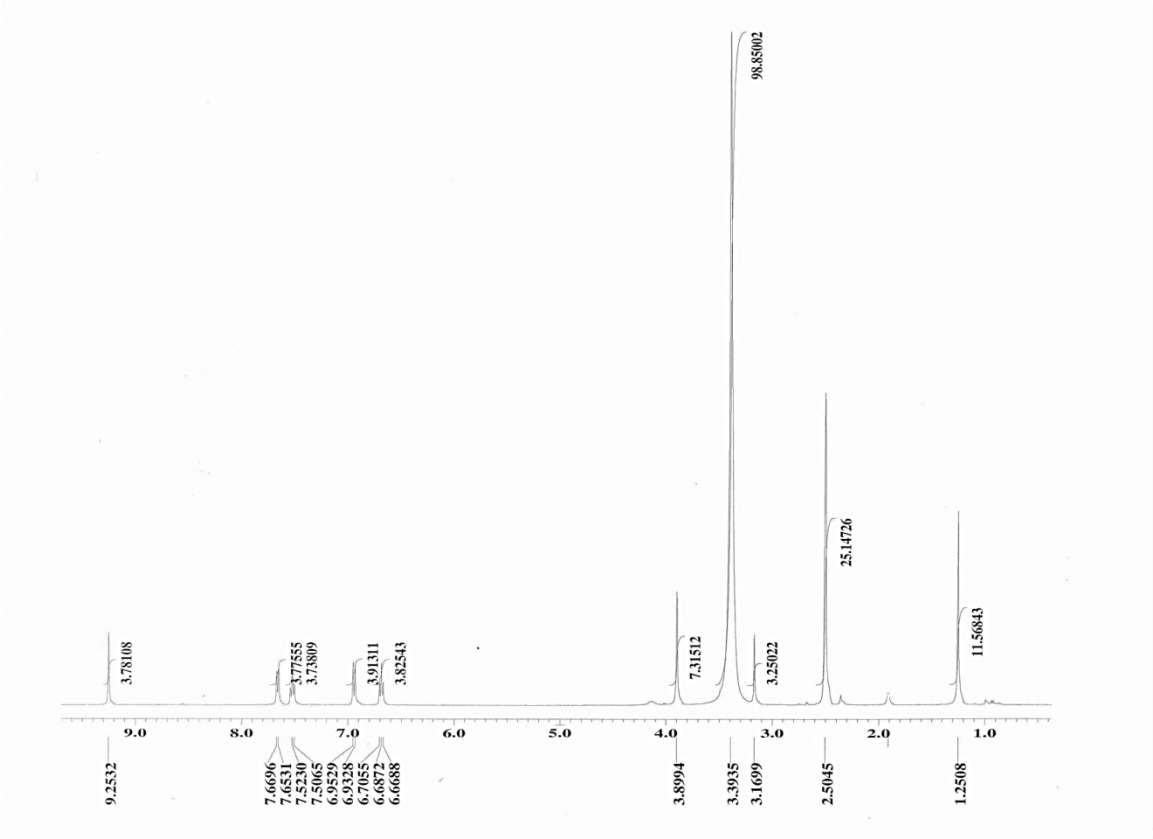

Fig 5S: ^{1}H NMR spectrum of Uranyl Complex

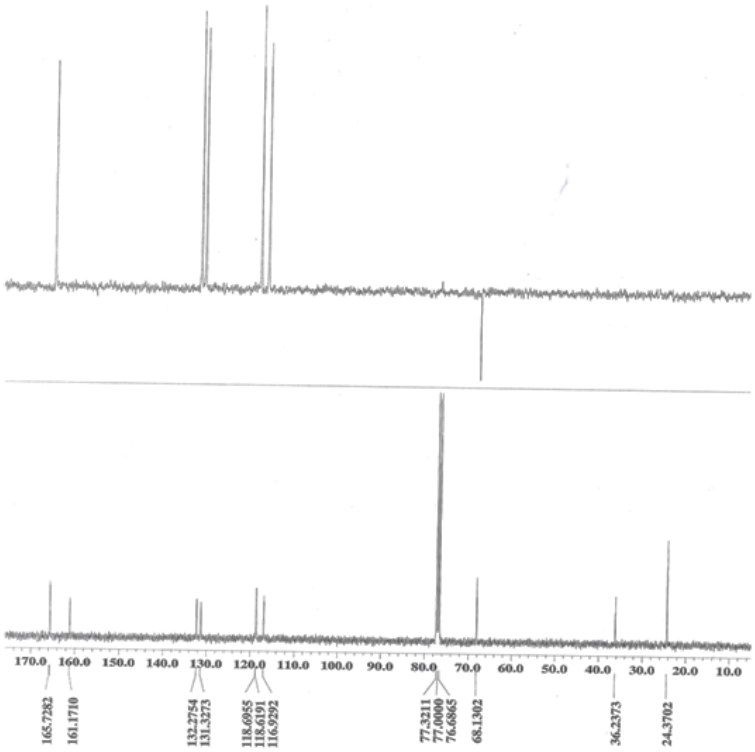

Fig 6S: DEPT-135 NMR of Ligand, H_2L

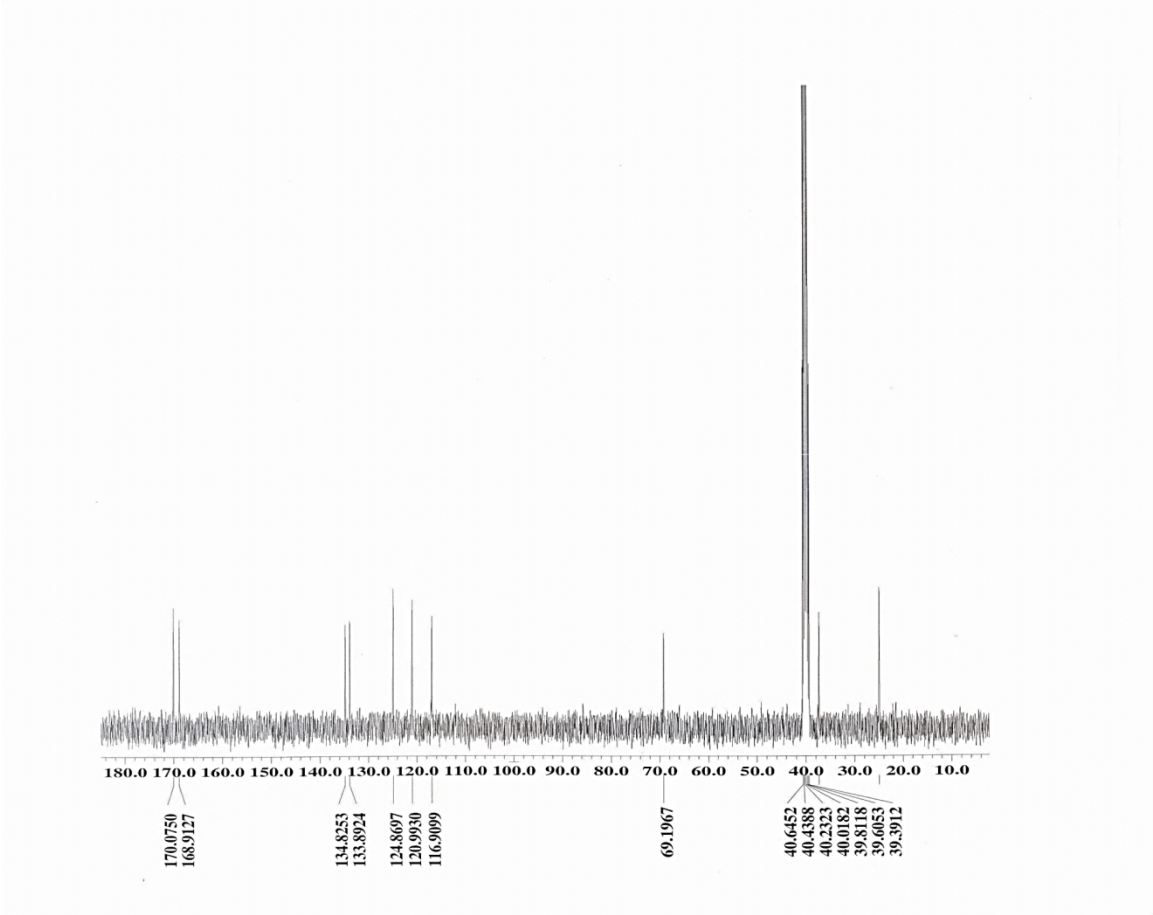

Fig 7S: ^{13}C NMR of Uranyl complex

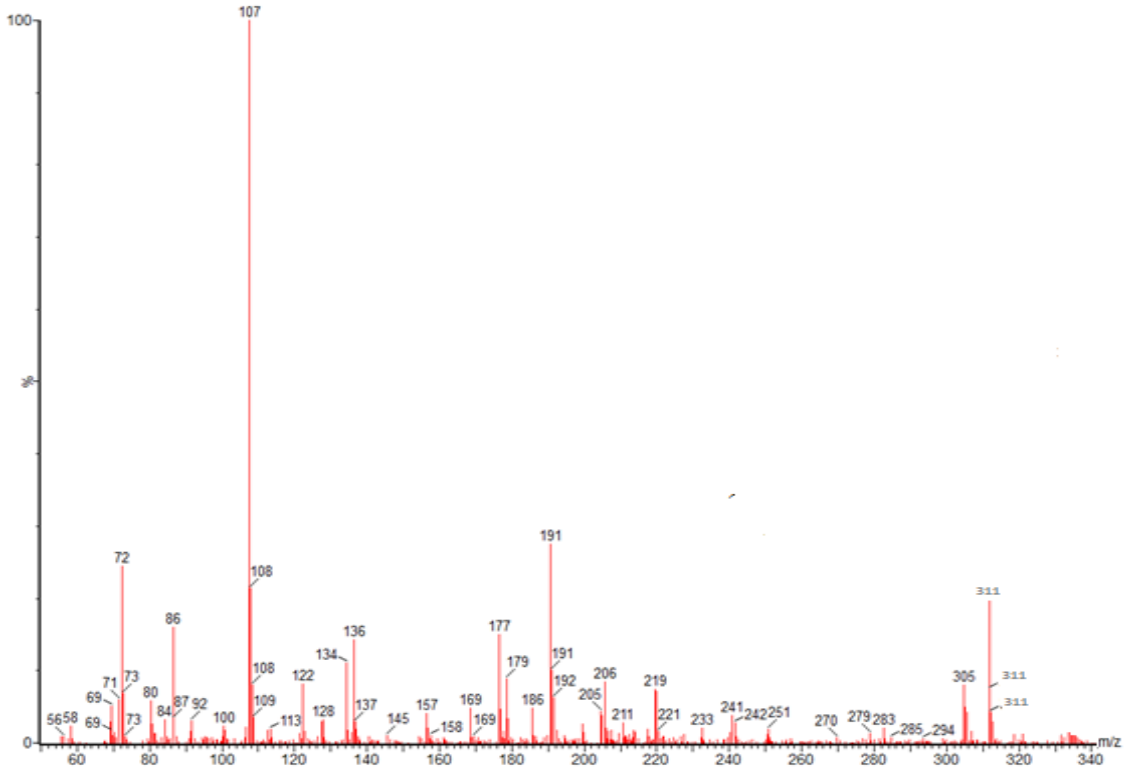

Fig 8S: ESI-MS Spectrum of ligand, H_2L

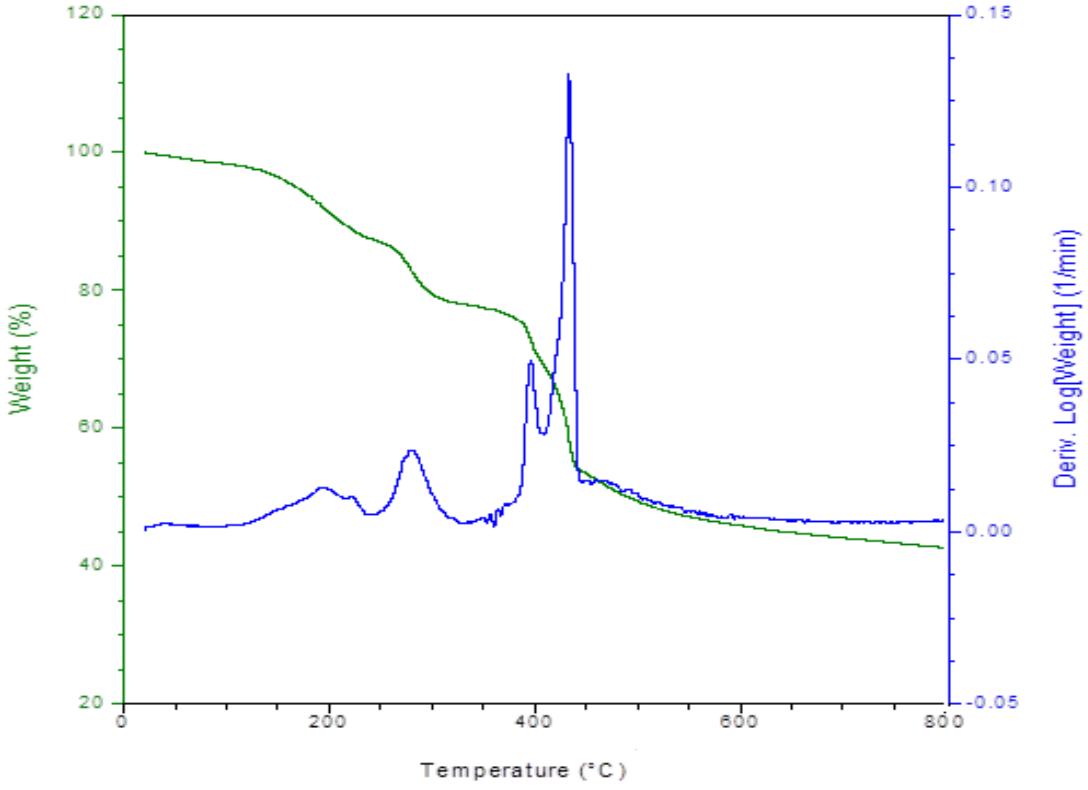

Fig 9S: TGA/DTA of Uranyl Complex

Table 1S.Crystal data and structure refinement for ligand, H_2L.

Empirical formula	C19 H22 N2 O2
Formula weight	310.39
Temperature	200(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P212121
Unit cell dimensions	a = 6.1281(3) A alpha = 90 deg. b = 15.9681(10) A beta = 90 deg. c = 17.3110(8) A gamma = 90 deg.
Volume	1693.95(16) A^3
Z, Calculated density	4, 1.217 Mg/m^3
Absorption coefficient	0.079 mm^-1
F(000)	664
Crystal size	0.40 x 0.25 x 0.04 mm
Theta range for data collection	2.55 to 27.00 deg.
Limiting indices	-7<=h<=7, -20<=k<=20, 20<=l<=22
Reflections collected / unique	18886 / 3681 [R(int) = 0.0439]
Completeness to theta = 27.00	99.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3681 / 0 / 218
Goodness-of-fit on F^2	1.067
Final R indices [I>2sigma(I)]	R1 = 0.0311, wR2 = 0.0772
R indices (all data)	R1 = 0.0367, wR2 = 0.0799
Largest diff. peak and hole	0.184 and -0.110 e.A^-3

Table 2S.Bond lengths [A] and angles [deg] for ligand, H_2L.

O(1)-C(1)	1.3524(17)	C(5)-C(6)	1.4008(18)
O(1)-H(1O)	0.91(2)	C(6)-C(7)	1.4626(17)
O(2)-C(8)	1.3512(16)	C(8)-C(9)	1.3961(19)
O(2)-H(2O)	0.96(2)	C(8)-C(13)	1.4086(18)
N(1)-C(7)	1.2788(17)	C(9)-C(10)	1.379(2)
N(1)-C(15)	1.4616(16)	C(10)-C(11)	1.385(2)
N(2)-C(14)	1.2747(17)	C(11)-C(12)	1.382(2)
N(2)-C(17)	1.4556(16)	C(12)-C(13)	1.3984(18)
C(1)-C(2)	1.3968(19)	C(13)-C(14)	1.4588(17)
C(1)-C(6)	1.4094(18)	C(15)-C(16)	1.5364(18)
C(2)-C(3)	1.374(2)	C(16)-C(19)	1.530(2)
C(3)-C(4)	1.385(2)	C(16)-C(18)	1.5353(17)
C(4)-C(5)	1.380(2)	C(16)-C(17)	1.5374(17)

C(1)-O(1)-H(1O)	106.3(12)	C(9)-C(8)-C(13)	119.54(12)
C(8)-O(2)-H(2O)	106.3(13)	C(10)-C(9)-C(8)	120.53(13)
C(7)-N(1)-C(15)	119.36(12)	C(9)-C(10)-C(11)	120.50(13)
C(14)-N(2)-C(17)	120.03(11)	C(12)-C(11)-C(10)	119.53(13)
O(1)-C(1)-C(2)	119.14(12)	C(11)-C(12)-C(13)	121.33(14)
O(1)-C(1)-C(6)	121.39(12)	C(12)-C(13)-C(8)	118.58(12)
C(2)-C(1)-C(6)	119.47(13)	C(12)-C(13)-C(14)	120.19(12)
C(3)-C(2)-C(1)	120.41(14)	C(8)-C(13)-C(14)	121.24(11)
C(2)-C(3)-C(4)	120.96(13)	N(2)-C(14)-C(13)	120.99(12)
C(5)-C(4)-C(3)	119.22(14)	N(1)-C(15)-C(16)	111.98(11)
C(4)-C(5)-C(6)	121.37(14)	C(19)-C(16)-C(18)	110.18(12)
C(5)-C(6)-C(1)	118.55(12)	C(19)-C(16)-C(15)	110.10(11)
C(5)-C(6)-C(7)	119.94(12)	C(18)-C(16)-C(15)	108.55(11)
C(1)-C(6)-C(7)	121.51(12)	C(19)-C(16)-C(17)	110.81(11)
N(1)-C(7)-C(6)	121.29(12)	C(18)-C(16)-C(17)	109.27(11)
O(2)-C(8)-C(9)	119.26(12)	C(15)-C(16)-C(17)	107.88(10)
O(2)-C(8)-C(13)	121.21(12)	N(2)-C(17)-C(16)	111.69(10)

Table 3S. Torsion angles [deg] for Uranyl complex.

O(4)-U(1)-O(1)-C(1)	36.7(3)
O(3)-U(1)-O(1)-C(1)	-142.1(3)
O(2)-U(1)-O(1)-C(1)	116.9(3)
O(5)-U(1)-O(1)-C(1)	131.3(3)
N(2)-U(1)-O(1)-C(1)	-44.7(3)
N(1)-U(1)-O(1)-C(1)	-55.9(3)
O(4)-U(1)-O(2)-C(8)	-140.5(3)
O(3)-U(1)-O(2)-C(8)	37.7(3)
O(1)-U(1)-O(2)-C(8)	139.5(3)
O(5)-U(1)-O(2)-C(8)	124.9(3)
N(2)-U(1)-O(2)-C(8)	-53.0(3)
N(1)-U(1)-O(2)-C(8)	-50.9(3)
O(4)-U(1)-O(5)-C(20)	-153.7(3)
O(3)-U(1)-O(5)-C(20)	25.0(3)
O(1)-U(1)-O(5)-C(20)	120.3(3)
O(2)-U(1)-O(5)-C(20)	-67.2(2)
N(2)-U(1)-O(5)-C(20)	-64.0(3)
N(1)-U(1)-O(5)-C(20)	107.9(3)
O(4)-U(1)-N(1)-C(7)	-60.7(3)
O(3)-U(1)-N(1)-C(7)	121.3(3)
O(1)-U(1)-N(1)-C(7)	25.6(2)
O(2)-U(1)-N(1)-C(7)	-148.9(2)
O(5)-U(1)-N(1)-C(7)	38.4(3)
N(2)-U(1)-N(1)-C(7)	-146.8(3)
O(4)-U(1)-N(1)-C(15)	122.6(2)
O(3)-U(1)-N(1)-C(15)	-55.4(2)

Table 4S**.** The calculated lowest-lying transitions of $[UO_2L(CH_3OH)]$ complex obtained using different functionals

	PBE1PBE	B3LYP	B3P86	CAM-B3LYP	M05	M06	M06-L	TPSSLYP1W	M11-L	Exp/nm
Peak 1	452.2	476.5	501.6	396.1	481.0	491.8	682.4	693.3	838.3	470
Peak 2	327.1	359.1	330.6	310.5	330.4	348.5	478.7	492.7	533.2	400
Peak 3	326.0	357.5	328.7	304.6	329.2	332.8	459.3	471.6	525.4	400

Table 5S.Second order perturbation interactions obtained for $[UO_2L(CH_3OH)]$ complex from NBO calculations

Donor (i)	Acceptor (j)	E(2) (kj mol^{-1})
n_{O5}	n^*_{U1}	96.24
n_{O4}	n^*_{U1}	81.59
n_{N8}	n^*_{U1}	37.83
n_{O4}	n^*_{U1}	35.25
π_{U1-O5}	π^*_{U1-O4}	23.37
$\pi_{C27-C29}$	$\pi^*_{C23-C25}$	21.97